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Design of Gradient Index Optical Thin Films

DISSERTATION

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DISSERTATION

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Doctor of Philosophy

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PREFACE

This research grew out of a desire to create a highly reflective multilayer film with very low resistance for vertical cavity surface emitting semiconductor lasers. The traditional cavity mirrors for these devices are formed by alternating layers of gallium arsenide and aluminum gallium arsenide. The abrupt changes in material which make a good mirror also make a poor conductor, so electrical pumping of these lasers is difficult. One solution is to design a mirror with no abrupt changes in material (lowering the resistance) while maintaining the high reflectance required for the laser cavity mirrors. In the course of the investigation, the original goal of designing, fabricating, and testing a vertical cavity laser device was found to be infeasible in the time available. My research therefore took a more theoretical path, and I decided to address the more general problem of gradient index thin film design.

I would like to express my thanks to my advisor, Maj Jeffrey Grantham, for his aid and support in my ever evolving dissertation. Dr Peter Haaland was also of great help during the development of the SWIFT algorithm. I would also like to thank Maj Gregory Warhola for his willingness to adopt me as my dissertation topic took a more mathematical turn. Finally, I wish to thank my wife Joan for her patience, understanding, and support throughout the years it took to complete my studies.

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ABSTRACT

Gradient index thin films provide greater flexibility for the design of optical coatings than the more conventional "layer" films. In addition, gradient index films have higher damage thresholds and better adhesion properties. In this dissertation I present an enhancement to the existing inverse Fourier transform gradient index design method, and develop a new optimal design method for gradient index films using a generalized Fourier series approach. The inverse Fourier transform method is modified to include use of the phase of the index profile as a variable in rugate filter design. Use of an optimal phase function in Fourier-based filter designs reduces the product of index contrast and thickness for desired reflectance spectra. The shape of the reflectance spectrum is recovered with greater fidelity by suppression of Gibbs oscillations and shifting of side-lobes into desired wavelength regions. A new method of gradient index thin film design using generalized Fourier series extends the domain of problems for which gradient index solutions can be found. The method is analogous to existing techniques for layer based coating design, but adds the flexibility of gradient index films. A subset of the coefficients of a generalized Fourier series representation of the gradient index of refraction profile are used as variables in a nonlinear constrained optimization formulation. The optimal values of the design coefficients are determined using a sequential quadratic programming algorithm. This method is particularly well suited for the design of coatings for laser applications, where only a few widely separated wavelength requirements exist. The generalized Fourier series method is extended to determine the minimum film thickness needed, as well as the index of refraction profile for the optimal film.

1. INTRODUCTION

1.1. Motivation

The Air Force is interested in optical thin film coatings for a variety of uses, including broad band anti-reflection coatings for low-observable applications, narrow pass filters for sensor protection, and high power laser mirrors. Most current thin film coatings are designed and constructed using a number of slabs of materials with different indices of refraction and thicknesses. The most popular method consists of alternating layers of high and low index material. The properties of the film are determined by the two index values used and the thicknesses of each layer in the film. Recently, there has been a growing interest in inhomogeneous or gradient index thin films, which are characterized by a continuously varying index of refraction throughout the film. The advantages of such gradient index films over the alternating stack type films are based on the elimination of the abrupt interfaces between materials. In a slab based design, very large electric fields can develop at the material interfaces. This can lead to damage of the film in high power laser applications [47:272]. Also, the current deposition methods demonstrate columnar growth patterns in each material. The columnar growth patterns create voids in the structure, which can increase scattering. In addition, the different material properties lead to large inherent stress between layers in the film [47:271-272]. Elimination of the interfaces by using gradient index designs promotes better adhesion to the substrate, reduces internal stress in the film, reduces scattering, and increases the damage threshold for the film [43:2864].

Several basic approaches to thin film design exist, including graphical, analytical, and digital design methods [11:97]. Digital techniques are of particular interest because

they can be used to design films with more complex properties than is possible analytically or graphically. Digital design techniques can be categorized as either refinement or synthesis techniques. Refinement techniques begin with an initial film design and iteratively refine it to achieve a better design. Synthesis techniques on the other hand generate a film design based on the desired film characteristics only. Several methods exist for both refinement of an initial design [11] or synthesis of a film [12]. One of the synthesis techniques relies on the inverse Fourier transform to relate the index of refraction of the film to the transmittance of the film. This technique, originally developed by Sossi and Kard [34,35,36], will be expanded upon in this work. In addition, new design techniques, based on a generalized Fourier series approach, will be developed.

The objective in designing a thin film is to take the performance requirements for the film and generate a design subject to constraints of available indices of refraction and acceptable total thickness. The performance requirements are usually stated as reflectance, transmittance, or absorption versus wavelength, incident polarization or angle. The conventional variables in the design are the number of layers in the film, and the index and/or thickness of each layer. For "simple" filters, such as notch or bandpass filters, anti-reflection coatings, and reflectors, designs by graphical methods or by knowledge of the properties of periodic multilayers are possible [12, 24]. Films with more complex properties require digital design methods.

1.2. Problem Statement

The purpose of this research is to create a design method to map between reflectivity and continuous index of refraction profiles that also allows for additional design constraints, such as limitations on the total film thickness and index of refraction

range. The process of designing an optical filter requires a mapping between the space of all possible index profiles and the space of all possible reflectivity characteristics. A mapping from index to reflectivity can be generated from Maxwell's equations. This mapping allows one to evaluate the performance characteristics of a film, in terms of reflectivity as a function of wavelength, angle of incidence, polarization, etc.. Unfortunately, this mapping is not invertible, so it cannot be used to design a film (except by trial and error). Most of the existing design techniques rely on the trial and error approach. The corrections to the index are based on numerical principles of optimal design theory. One exception to this approach is the inverse Fourier transform technique. This design method is derived from Maxwell's equations by making several approximations. However, this method maps one reflectivity profile to many possible index profiles. In addition, there is no mechanism to impose additional constraints on the design, such as available index range or total thickness.

This research is presented in two phases. The first phase is to investigate design of gradient index thin films by the inverse Fourier transform method. The second phase is to create a new method for solving the inverse problem of identifying an index of refraction profile for a given reflectivity, based on a generalized Fourier series approach. Two variations on this theme are explored: a Fourier series method and a wavelet method. The wavelets provide a different framework for analyzing the structure of the index of refraction. A wavelet decomposition of a "signal" is analogous to a Fourier series decomposition, but the information is packaged in terms of "scale" and "shift", rather than the more familiar frequency and phase. Another reason to use wavelets is that each wavelet has a finite extent, as opposed to the sines and cosines of Fourier series. This finite support is helpful because it allows one to focus only on the elements of the design that are important. As an example, the inverse Fourier transform method requires the user to specify the reflectivity over a broader range than the design requirements specify. This

is required to achieve sufficient detail in the index of refraction profile. This forces the design to meet more stringent conditions than are really needed. The finite support of the wavelets should allow one to overcome such problems. The theory and concepts of this wavelet formalism are presented in more detail in Appendix C.

1.3. Organization

Chapter 2 presents background information on existing thin film design techniques and the basic theory of thin films. Chapter 3 discusses the inverse Fourier transform method for synthesis of thin films, as well as a modification to the existing theory allowing optimal synthesis of a thin film. Chapter 4 discusses optimal design of gradient index films using Fourier series and wavelet series. The final chapter summarizes the dissertation and presents suggestions for future research in this area. The appendices include an explanation of the numerical considerations involved in implementing the inverse Fourier transform techniques of Chapter 3 (Appendix A), a brief outline of optimization theory (Appendix B), the wavelet theory needed in this research (Appendix C), and the programs used in this work (Appendix D).

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3. VITA

Captain Jeffrey J. Druessel was born on 15 October, 1963 in Decatur, Illinois. He graduated from Stephen Decatur High School in Decatur, Illinois in 1981, and continued his education at the University of Illinois at Urbana, Illinois, graduating in 1985 with a Bachelor of Science degree in Engineering Physics. He was commissioned in the United States Air Force in 1986 and was stationed at Vandenberg AFB, CA. During this tour he served as a weapons systems analyst for development testing of the Air Launched Anti-Satellite Missile, the Strategic Defense Initiative Space Based Interceptor Program, and the Peacekeeper and Small Intercontinental Ballistic missiles. In addition, he attended the University of Southern California extension at Vandenberg AFB, and graduated with a Master of Science in Systems Management in 1988. He married the former Joan M. Cairns of Lompoc, CA in April 1988. He entered the Air Force Institute of Technology School of Engineering in May 1990, and graduated with a Master of Science degree in Engineering Physics in 1991.

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2. Background

This chapter presents the historical background of thin film design methods and the current state of the art for gradient index film design and fabrication. In addition, the basic theory of optical properties of thin films necessary for the analysis and synthesis of thin films is presented.

2.1. Historical Perspective

To appreciate the significance of the new approach to gradient index thin film design presented in this dissertation, a brief history of thin film design techniques is needed. Thin films were first discovered in the late 1600's by Robert Hooke and Sir Isaac Newton in the phenomenon known as "Newton's rings" [19:299,24:2]. The first anti-reflection coatings were made by Fraunhofer in 1817 [24:2]. The modern era of thin film manufacturing began in the 1930's, with the invention of reliable vapor deposition techniques [24:4].

Modern design techniques can be broken into three broad categories; analytical methods, graphical methods, and digital designs. Analytical techniques use a few simple elements as building blocks to design more complex filters. The building blocks used, such as quarter wave stacks, are selected because the relationship between the few variables of the basic element (i.e., index, thickness, number of layers) and the reflectivity (i.e., total reflectivity, pass band width, stop band location) are well known. A specific design is then created by combining a series of these building blocks until the desired profile is obtained [24:164-172]. This technique is effective for fairly simple designs, such as a bandpass filter, but does not work as well for more complex designs. Many of the existing thin film

design techniques rely on the intuition of the designer, based on his experience with basic elements of the design. One example of this is the design of bandpass filters from quarter wave stacks [24:164-172]. Another example is the design of rugate filters, where the basic building blocks are sinusoids [22]. It has been noted that one of the standard rugate filter profiles for a bandpass filter bears a remarkable resemblance to a Morlet wavelet [37].

Graphical techniques are closely related to the analytical methods described above. They consist of various methods to simplify the calculations necessary in the analytical method by graphing the relationships between the variables. Examples of these techniques include the Smith chart, reflection circles, and admittance loci [24:54-66].

The techniques of primary interest here are the digital design methods. Digital design methods can be further subdivided into two categories; refinement and synthesis techniques. Refinement techniques are characterized by the fact that they require an initial starting design. Synthesis techniques, on the other hand, create their design without an initial guess [11: 2876]. There are over a dozen published refinement methods, and about half a dozen synthesis methods. There are undoubtedly many more unpublished design methods that are proprietary to the thin film manufacturing companies. Most of the methods make use of a merit function, which is a measure of how close the existing design is to the desired result. Some of the methods are capable of locating a global minimum, which is the true optimal solution to the problem. Other methods only solve for local minima based on the initial guess. Brief descriptions of a few of the published design methods are given below.

Refinement Methods: [11:2878-2882]

1. *Adaptive Random Search*: This procedure takes a starting design and applies a random change to the parameters of the design. The results at each step are compared to the desired result through a merit function. Changes in the design that reduce the merit

function are kept, while others are discarded. The magnitude of the change in parameters is also changed at each step, making this procedure perform both a local and global search. This means that if the "best" design is very different from the starting design, this method may find it. Local search methods only make small changes to the initial design. This method stops its iteration when the merit function passes a preset threshold or the method stops converging

2. *Damped Least Squares*: This method uses the derivatives of the quantities of interest in the merit function with respect to the construction parameters to determine the changes to be made to the design. Since the design problem is highly non-linear, the size of the change in any one step is limited by a damped least squares algorithm. This method performs a local search from the starting design.

3. *Golden Section Method*: The golden section method takes an initial design and varies each of the construction parameters in sequence. The optimal value for each parameter is found, (within the preset limits for each) before continuing on to change the next parameter. This algorithm converges fairly rapidly, and can find solutions far from the initial design.

4. *Hookes and Jeeves Pattern Search*: This technique is composed of two steps; an exploration and a pattern search. The exploration is to change each parameter up and down by a small amount, and determine which changes improve the merit function. The pattern search extrapolates in the direction of improvement from the exploration step. The step sizes are changed, and then the process is repeated. The process stops when the change in the merit function is smaller than a preset limit.

5. *Simulated Annealing*: The physical process of annealing is heating a sample and allowing the molecules to find a minimum energy state during cooling. This idea is used mathematically in this design approach. This method can deal with arbitrarily large numbers of design parameters, and can find globally optimal solutions.

Synthesis Methods: [23:3790-3791]

1. *Comprehensive Search Method*: This method is limited to films with only a few layers (<6). The global optimal solution is found by testing every possible combination of index and thickness allowed. Clearly, only a limited number of indices and thickness can be used. The advantage of this method is that it finds the truly optimal solution given the constraints on index and thickness. The disadvantage is it takes so much computer time to check every possible combination that only very simple systems can be designed this way.

2. *Gradual-Evolution Method*: This method is a modification of the comprehensive search described above. Instead of designing the whole film in one step, a smaller design, say three layers, is done by comprehensive search. The result is then added as part of the substrate, and an additional few layers are designed on this "new" substrate, again by comprehensive search. Since only a few layers are changed at a time, this method is much faster than the full comprehensive search method. However, there is no longer a guarantee that the global optimal solution will be found.

3. *Minus Filter Method*: A minus filter is a design that transmits all incident radiation except that in a narrow spectral band. Thelen has shown that all dielectric minus filters can be made using quarter wave stacks with several indices of refraction [39:365-369]. This design technique breaks the desired reflectivity profile into several minus filters, and then places the individual designs in series.

4. *Flip-Flop Method*: This unique approach uses many thin layers and only two indices of refraction. The algorithm is to pass through the film in sequences, flipping each layer between high and low index and calculating the resultant merit function. After several passes through the film, this method converges on a solution. The advantage to this technique is it uses only two materials, which is preferred by manufacturers, and it requires no initial design. The method sometimes results in alternating very thin layers, but this can usually be corrected manually later.

2.2. Gradient Index Film Design and Fabrication

The current gradient index film design techniques focus on the inverse Fourier transform method and the rugate film design method. The inverse Fourier transform method can be classified as a synthesis technique, since no initial design is required. The rugate design method is an analytical design technique.

1. *Inverse Fourier Transform Method:* The use of Fourier transforms in the synthesis of thin films was first proposed by Delano in 1967 [9]. Sossi is generally credited with the development of the inverse Fourier transform method for thin film design [34,35,36]. Sossi's papers introduce a Fourier transform relationship between the logarithmic derivative of index of refraction and the reflectance of the film. This design technique was further developed by Dobrowolski and Lowe in 1978 [10]. Many authors have applied this method to various design problems, and offered modifications to the theory to better suit their needs. These include design of wideband anti-reflectance coatings [44] and high reflectance filters [16,43]. Other work has focused on modifying the theory of the method to improve the quality of the results or ease of computation [4,6,14,42]. This method, along with a modification of my design, will be described in detail in Section 3.2 below.

2. *Rugate Design Method:* A rugate filter is composed of a number of basic elements combined to achieve the desired optical properties of the film. The fundamental rugate design element is a sine wave refractive index profile on a substrate [22]. The basic rugate film has a notch reflectance profile, with the location, width, and height of the notch controlled by five parameters. More complicated rugate films are created by adding several basic rugates in parallel or in series, and including apodization functions or matching layers to suppress sidebands in the reflectance.

The fabrication of films designed using these techniques is done in one of two ways. The first way is to use the concept of the Herpin equivalent index to convert a gradient index design into a two index material system, and make an equivalent film out of discrete layers [3,15,24:191-200]. This method allows the use of gradient index design methods to design conventional alternating layer based films, but does not offer the advantages an actual gradient index film would. The other fabrication possibility is to deposit the gradient index profile as designed. This is currently on the forefront of existing technology, and is an active area of research. There are several material systems that can be used to produce gradient index profiles. Table 2-1 lists some of the materials available, along with the index range and literature reference for additional information.

Table 2-1: Gradient Index Film Materials

Material System	Index Range	Reference
$\text{Ge}_{1-x}\text{S}_x$	3.5 - 4.0	[22:97]
$\text{Al}_{1-x}\text{Ga}_x\text{As}$	2.9 - 3.6	[33:588]
$\text{ZnS}_{1-x}\text{Se}_x$	2.2 - 2.5	[22:97]
SiO_xN_y	1.5 - 2.0	[22:97, 29:179]
$\text{SiO}_2 - \text{Ta}_2\text{O}_5$	1.65 - 2.0	[1:141-145]
$\text{MgF}_2 - \text{TiO}_2$	1.38 - 2.3	[41:189-196]
$\text{CeF}_3 - \text{ZnS}$	1.6 - 2.2	[20:61]
$\text{MgF}_2 - \text{ZnSe}$	1.38 - 2.5	[20:197-204]

2.3. Optical Properties of Thin Films

This section presents the theory and methods for determining the reflectance properties of a film. The first section presents the derivation of the reflectance from Maxwell's equations, and the second section outlines the implementation of this formulation for a single thin film. The third section extends this implementation to gradient index films.

2.3.1. Derivation of Reflectance

This section presents the formal derivation for determining the reflectance of a film starting from Maxwell's equations. Figure 2.1 shows the coordinates used in the derivation. The surface of the film is the x - y plane, and the physical thickness of the film is along z . The origin is at the film-substrate interface, and the thickness of the film is denoted by L .

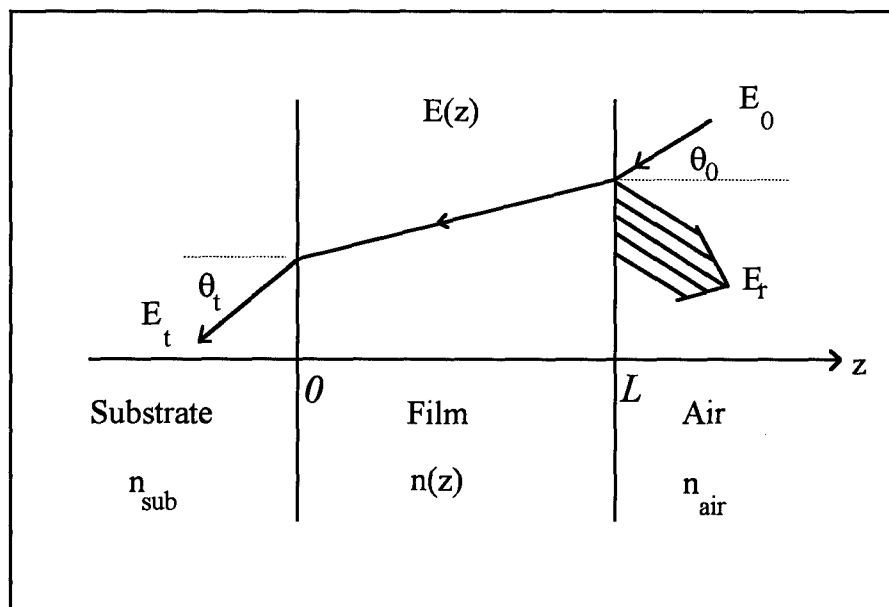


Figure 2.1: Geometry of Thin Film

Assuming a time dependence of $\exp[i\omega t]$, Maxwell's equations in SI units are

$$\begin{aligned} \text{curl } \vec{H} &= i\omega \epsilon \vec{E} \\ \text{curl } \vec{E} &= -i\omega \mu \vec{H} \\ \text{div } \vec{E} &= 0 \\ \text{div } \vec{H} &= 0 \end{aligned} \quad (2.1)$$

where E is the electric field, H is the magnetic field, ϵ is the permittivity, and μ is the permeability.

Two polarizations must be considered to determine the electric field; the transverse electric (TE) case, which has its electric field aligned perpendicular to the plane of incidence, and the transverse magnetic (TM) case, which has its electric field aligned parallel to the plane of incidence. By the symmetry of Maxwell's equations, the TM case can be deduced from the TE case with a substitution of E for H and ϵ for μ . The plane of incidence is defined by the direction of propagation of the incident light and the normal to the surface. Define the x direction as the direction in which the electric field is aligned, so the fields can be written as

$$\vec{E} = \begin{bmatrix} E_x(z) \exp[i\omega t - ikSy] \\ 0 \\ 0 \end{bmatrix} \quad \vec{H} = \begin{bmatrix} 0 \\ H_y(z) \exp[i\omega t - ikSy] \\ H_z(z) \exp[i\omega t - ikSy] \end{bmatrix} \quad (2.2)$$

Here S is an invariant, $S = n_0 \sin(\theta_0)$, where n_0 is the index of refraction of the incident medium, and θ_0 is the angle of incidence. Also, ω is the frequency of the incident light, k is the wave number of the light, $k=2\pi/\lambda$, and λ is the wavelength in vacuum. Substituting these expressions for E and H into Maxwell's equations yields

$$\begin{aligned}
Z_0 \frac{\partial H_y(z)}{\partial z} &= -ik \left(\epsilon_r - \frac{S^2}{\mu_r} \right) E_x(z) \\
\frac{\partial E_x(z)}{\partial z} &= -ik \mu_r Z_0 H_y(z) \\
H_z(z) &= - \left(\frac{S}{Z_0 \mu_r} \right) E_x(z)
\end{aligned} \tag{2.3}$$

where Z_0 is the impedance of free space, $Z_0 = \sqrt{\mu_0/\epsilon_0}$, and

ϵ_0, μ_0 are the permittivity and permeability of free space,

ϵ_r, μ_r are the relative permittivity and permeability of the medium.

Let $N^2(z) = \epsilon_r(z)\mu_r - S^2$, and consider only dielectric materials with $\mu_r=1$. $N(z)$ is always a real valued function since $S < 1$ for all cases considered here and $\epsilon_r > 1$ for all dielectric materials. For normal incidence, $S=0$, and N reduces to the usual definition of index of refraction. Also define two new complex valued variables u and v by

$$u(z) = \frac{E_x(z)}{E_t} \quad v(z) = -\mu_r Z_0 \frac{H_y(z)}{E_t} \tag{2.4}$$

The normalization factor E_t is the complex amplitude of the transmitted wave. Using the new normalized field variables, Maxwell's equations reduce to the following pair of coupled first order ordinary differential equations

$$u'(z) = ikv(z) \quad \text{and} \quad v'(z) = ik N^2(z)u(z) \tag{2.5}$$

with boundary conditions

$$u(0) = 1 \quad v(0) = -n_{sub} \cos(\theta_i) \tag{2.6}$$

In this formulation, the amplitude reflectance and transmittance of the film, $r(k)$ and $t(k)$ respectively, are found from the Fresnel equations: [40:4274]

$$r(k) = \frac{n_{air}u(L, k) \cos(\theta_0) + v(L, k) \cos(\theta_t)}{n_{air}u(L, k) \cos(\theta_0) - v(L, k) \cos(\theta_t)} \quad (2.7)$$

$$t(k) = \frac{2n_{air}u(L, k) \cos(\theta_0)}{n_{air}u(L, k) \cos(\theta_0) - v(L, k) \cos(\theta_t)}$$

Here the field variable dependence on the wave number k has been called out explicitly.

2.3.2. Multilayer Thin Films

The optical properties of a multilayer thin film are based upon the Fresnel reflection at interfaces and the interference between multiple reflections. The reflectance of such a film can be determined by using Maxwell's equations and applying the boundary conditions at both interfaces. MacLeod has shown the fields at the first interface are related to the fields at the second interface by [24:35]

$$\begin{bmatrix} E_{01} \\ H_{01} \end{bmatrix} = \begin{bmatrix} \cos(\delta) & i \sin(\delta)/\eta_1 \\ i \eta_1 \sin(\delta) & \cos(\delta) \end{bmatrix} \begin{bmatrix} E_{12} \\ H_{12} \end{bmatrix} \quad (2.8)$$

where E_{01} , H_{01} represent the field at the interface between the incident media and the film, and E_{12} , H_{12} represent the field at the interface between film and the substrate. The optical admittance of the film material η is given by

$$\begin{aligned}
\eta_1 = H_1/E_1 &= \frac{n_1 Y_0}{\cos(\theta)} & TM \\
&= n_1 Y_0 \cos(\theta) & TE
\end{aligned} \tag{2.9}$$

with $Y_0=1/377$ Siemens. The phase shift δ is given by

$$\delta = 2\pi n_1 d \cos(\theta)/\lambda \tag{2.10}$$

where n_1 is the index of refraction of the film, d is the thickness of the film, θ is the angle between the direction of propagation and the normal to the surface of the film, and λ is the wavelength in vacuum. Note that the phase shift δ can be complex, and the angle θ_1 , found using Snell's Law, may also be complex. The complex amplitude reflectivity, ρ , and the real intensity reflectance, R , can be found from Equation 2.8 by defining an input optical admittance for the assembly as

$$Y \equiv H_{01}/E_{01} \tag{2.11}$$

Then for an incident medium with an optical admittance of η_0

$$\begin{aligned}
\rho &= \frac{\eta_0 - Y}{\eta_0 + Y} \\
R &= \left(\frac{\eta_0 - Y}{\eta_0 + Y} \right) \left(\frac{\eta_0 - Y}{\eta_0 + Y} \right)^*
\end{aligned} \tag{2.12}$$

where the asterisk indicates complex conjugation.

Since the reflectance depends only on the optical admittance of the film, Y , rearrange Equation 2.8 to find Y :

$$\begin{bmatrix} B \\ C \end{bmatrix} = \begin{bmatrix} \cos(\delta) & i \sin(\delta) / \eta_1 \\ i \eta_1 \sin(\delta) & \cos(\delta) \end{bmatrix} \begin{bmatrix} 1 \\ \eta_2 \end{bmatrix} \quad (2.13)$$

$$Y = C/B$$

The matrix above is the characteristic matrix for the film, and depends only on the film materials and the angle of incidence of the impinging light. This matrix technique can be directly extended to an assembly of many thin films. So, given q thin film layers, each with specified index and thickness, the characteristic matrix of the assembly is given by

$$\begin{bmatrix} B \\ C \end{bmatrix} = \prod_{r=1}^q \begin{bmatrix} \cos(\delta_r) & i \sin(\delta_r) / \eta_r \\ i \eta_r \sin(\delta_r) & \cos(\delta_r) \end{bmatrix} \begin{bmatrix} 1 \\ \eta_s \end{bmatrix} \quad (2.14)$$

where for each layer r the phase shift δ_r is

$$\delta_r = 2\pi n_r d_r \cos(\theta_r) / \lambda \quad (2.15)$$

and n_r is the index of refraction of the layer, d_r is the thickness of the layer, and the angle θ_r is found using Snell's Law. These equations form the basis for the design of thin film dielectric mirrors.

In addition to determining the reflectivity of a multilayer thin film, the characteristic matrix above can also be used to determine the phase of the reflected field. Writing the optical admittance of the film as $Y = a + bi$, the phase, ϕ , of the field upon reflection is given by [24:37]

$$\tan(\phi) = \frac{-2b\eta_0}{(\eta_0^2 - a^2 - b^2)} \quad (2.16)$$

The simplest example of a mirror using these multilayer films is a quarter wave stack. This is a series of layers each with an optical thickness of one quarter of the wavelength of the incident light. If the index and thickness of each layer are chosen so the optical path length $nd = \lambda/4$, and the light is at normal incidence, the phase shift δ for each layer is $\pi/2$. The characteristic matrix then reduces to

$$\begin{bmatrix} B \\ C \end{bmatrix} = \prod_{r=1}^q \begin{bmatrix} 0 & i/\eta_r \\ i\eta_r & 0 \end{bmatrix} \begin{bmatrix} 1 \\ \eta_s \end{bmatrix} \quad (2.17)$$

This characteristic matrix is very easy to calculate. An example of such a quarter wave stack is 25 alternating layers of GaAs and AlAs on a GaAs substrate, which have indices of refraction of 3.6 and 3.2 respectively [33:588]. If the design wavelength is 1.0 micron, this mirror is 93.6% reflective at this center wavelength and has a reflectivity versus wavelength profile as shown in Figure 2.2.

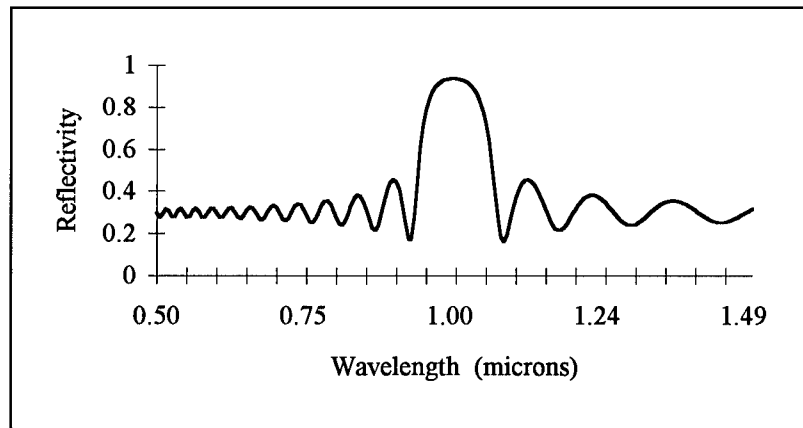


Figure 2.2: Reflectivity vs. wavelength for 25 layer quarter wave stack of GaAs/AlAs on a GaAs substrate.

2.3.3. Gradient Index Films

The analysis above assumes the mirror is formed by a discrete number of layers with well-defined thickness and index of refraction. How does one treat a structure where the index varies continuously? One approach, derived by Bovard, is to start from the beginning with Maxwell's equations and develop an expression for the characteristic matrix of the film based on the known index of refraction as a function of position in the film [4:1999-2001]. Unfortunately, the resultant expression contains an infinite series of integrals, which makes evaluation impracticable. Another alternative, and the one implemented here (see **REFLECT.M** in Appendix D), is to approximate the continuous film as a discrete film with many small layers. As a general rule, discrete layers on the order of 5 nm thick give a good approximation for the reflectance of a gradient index film for visible light [6:5429]. Since the formalism presented above includes the complex portion of the fields involved, the interference effects are already incorporated in the calculation. This is of critical importance to the validity of this approach, since high reflectivity depends on destructive interference of the transmitted fields.

The reflectance is calculated by a "C" language version of **REFLECT.M**. The conversion of this program from the MATLAB™ language to "C" increases the speed of each reflectance calculation by at least a factor of ten. The "C" language program, **REFLECT.C**, is also included in Appendix D. The inputs to **REFLECT.C** are the sampled values of the index, the substrate index, the vector of wavenumbers k at which to determine the reflectance, and the array of sample positions in the film x . The output is an array of reflectances, one for each of the input wavenumbers k . The units for x and k must be consistent, i.e. microns and inverse microns or nanometers and inverse nanometers. The programs **REFLECT.M** and **REFLECT.C** are used throughout the dissertation to determine the reflectance characteristics of the gradient index thin film designs.

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4. Vita

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Figure 2.1: Geometry of Thin Film 11

Figure 2.2: Reflectivity vs. wavelength for 25 layer quarter wave stack of GaAs/AlAs on a GaAs substrate. 17

Table 2-1: Gradient Index Film Materials 10

Appendix A : SWIFT Numerical Design Considerations

The discrete implementation of the inverse Fourier transform relation in Equation 3.1 is accomplished using the fast Fourier transform (FFT) algorithm in the MATLAB™ programming environment. MATLAB™ is a “technical computing environment for high-performance numeric computation and visualization” [27:i], which includes a high level programming capability. The MATLAB™ programs developed for this work are included in Appendix D. The implementation of the SWIFT technique is done using two programs: **QUE.M** and **SWIFT.M**. The program **QUE.M** uses a valid expression for $Q(k)$ such as one of the forms of Equation 3.11 to generate a sampled version of $Q(k)/k$ for notch reflectance profiles. **SWIFT.M** calculates the phase function for given $Q(k)/k$ using the SWIFT technique (Equations 3.13 and 3.18), and then calculates the index profile using the built in inverse Fourier transform (Equation 3.1). This program numerically estimates the integral in Equation 3.18 from the sampled values of $Q(k)$ using a simple trapezoid summation algorithm. A third program, **REFLECT.M**, is used to estimate the reflectance for a gradient index film by approximating the film by thin, homogeneous layers at each sample index value and implementing Equations 2.12 through 2.15.

The inputs to **QUE.M** are the lower and upper wavelength limits for the notch reflector in microns, the reflectivity of the notch (between 0 and 1), the number of samples to use, and the total thickness of the film to model in microns. Note that the total thickness of the film here is not the same as the desired film thickness, nor the “power spread” thickness of the SWIFT theory. The relationship among these three design parameters will be further discussed below. The functional dependence of $Q(k)$ on the reflectivity or transmission of the film (such as in Equation 3.11) is hard coded in the

program. The output of the **QUE.M** program is a vector containing the samples values of $Q(k)/k$.

The inputs to the **SWIFT.M** program are the vector of $Q(k)/k$ values output by **QUE.M**, the number of samples, the lower and upper wavelength values in microns used to generate the Q function, the total film thickness, and the "power spread" thickness for the SWIFT algorithm. Again, this need not be the same as the desired film thickness. The output of the program is a matrix; the first column contains the sample values of the index, the second column contains the optical thickness of that layer, and the third column is the position of the sample in optical thickness.

The inputs to the **REFLECT.M** program are the index matrix of index values and layer thicknesses from **SWIFT.M**, and the number of plot points. The index of the substrate and exit medium are fixed in the code, as is the wavelength range to calculate. The output is a matrix with the reflectance in column one and the wavelength in microns in column two.

There are a few numerical computation issues associated with using the discrete implementation of the Fourier transform. The functions **QUE.M** and **SWIFT.M** above require the user to define the sampling scheme to use in the Fourier transform calculation. The goal is to accurately specify an index of refraction profile over some finite thickness of film. There are several related parameters that must be specified to calculate a discrete Fourier transform. Note that the Fourier transform variables in the theory are the double optical thickness, x , of the index of refraction and the wavenumber, k , of the Q function. However, the reflectance calculation requires the index profile be specified in terms of optical thickness. For consistency, all thicknesses specified as inputs to and outputs from the programs are in optical thickness, and the conversion to double optical thickness is done inside the programs as necessary.

The parameters for the index profile are: number of sample values, denoted by N_s , the spacing of samples in optical thickness, denoted by Δ , the total optical thickness of the film sampled, d_{Total} , and the design optical thickness of the film, d_{film} . The parameters for the Q function in k -space are: the number of samples, N_s , the spacing of samples, $\delta = 1/(d_{Total})$, and the total range of k -space sampled, $1/(\Delta)$. Clearly, the number of samples can be found from the simple relation: $N_s = d_{Total}/\Delta$. The critical frequency, or Nyquist frequency, is related to the sample spacing of the index by $f_c = 1/(2\Delta)$. The various parameters for specifying the numerical sampling are illustrated in Figure A.1 below. The sampling densities actually used for calculation are much higher than depicted in this figure. The method for determining the sampling density needed is illustrated in the example below. All the examples in Section 3.3 use the same approach.

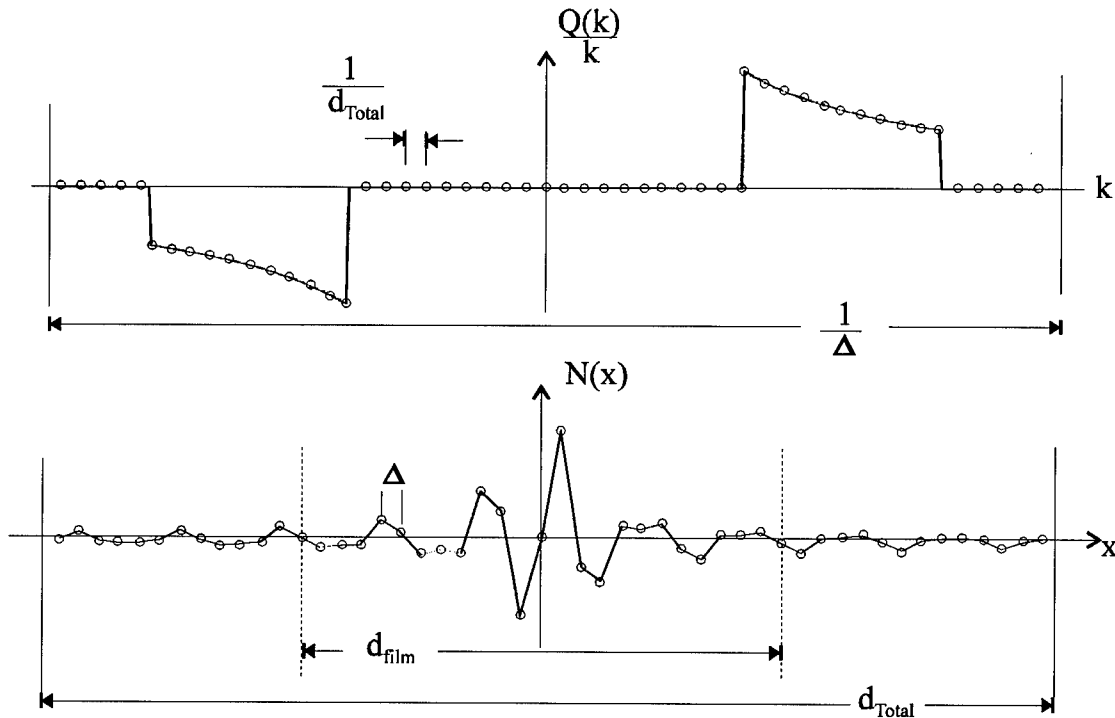


Figure A.1: Illustration of numerical parameters for discrete Fourier transform.

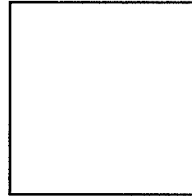
Acceptable values for the design parameters are found by considering the physical constraints on the design problem. First, the number of samples, N_s , should be a power of two to take advantage of the efficiency of the fast Fourier transform algorithm. The sample spacing of the index of refraction profile, Δ , should be on the order of one sample every five nm, to ensure the reflectivity calculation is accurate. Also, the Q function, which is the starting point for this design, must be adequately sampled. The number of non-zero samples of the Q function is denoted by N_0 . Finally, the total spatial thickness of the film, d_{Total} , must be sufficiently large to minimize spatial aliasing in the index. Aliasing arises from the finite sampling of a function. Any power that lies outside the Nyquist range is folded back inside the range, generating in this case an inverse Fourier transform that is incorrect [30:387]. Viewed another way, this means that the sampling of the Q function must be sufficiently high to insure the index profile calculated is near the substrate value at the edges of the film.

To illustrate the process to determine acceptable parameter values for a problem, the parameters for the first example in Section 3.3.1 will be found below. Recall this example is to design a narrow-band reflectance filter with a reflectivity of 90% from the lower (initial) design wavelength, $\lambda_i=580$, to the upper (final) design wavelength, $\lambda_f=620$ nm, and 0% outside this band. The indices of the substrate and the incident medium are the same ($n_{sub} = n_{out} = 1.50$). The desired optical thickness of the film is $d_{film}=30$ μm . The numerical parameters for the sampling are found by requiring the index sample spacing, Δ , to be on the order of five nm in optical thickness, the number of non-zero samples, N_0 , of the Q function to be about 25, and the total number of samples, N_s , to be a power of two. The first step in determining appropriate parameter values is to make a rough estimate, based on the values above. The second step will be to evaluate the numerical values produced, and then select a set of new numerical values that satisfy all the constraints.

First, since the sample spacing in k -space is the inverse of the total thickness (see Figure A.1), the requirement for 25 non-zero samples of the Q function over notch design wavelengths can be used to determine the total double optical thickness:

$$d_{Total} = \frac{N_0}{\frac{1}{\lambda_i} - \frac{1}{\lambda_f}} = \frac{25}{\frac{1}{0.58} - \frac{1}{0.62}} = 225 \mu\text{m} \quad (\text{A.1})$$

Note that for this calculation the spatial frequencies are defined as $1/\lambda$, rather than $2\pi/\lambda$. This is to be consistent with the QUE.M and SWIFT.M programs in Appendix D. This value for d_{Total} can be used along with the sample spacing, Δ , of the index profile to estimate the number of samples needed, N_s . The sample spacing, Δ , must be multiplied by a factor of 2 to convert the requirement on the sample spacing in the index from optical thickness (required by the reflectance calculation program) to double optical thickness, which is the variable of the Fourier transform relation. The sample spacing value to use in these calculations is therefore $\Delta=2(0.005)=0.010 \mu\text{m}$.



(A.2)

At this point, constrain the number of samples, N_s , to be a power of two. Unfortunately, the N_s found above is not a power of two, and the closest powers of 2 are $2^{14}=16,384$, and $2^{15}=32,768$. In the interest of minimizing computation time, choose the lower number of samples, and then determine the impact on the other parameters. So, for $N_s=2^{14}=16,384$, and keeping the original desired sample spacing in double optical path length, $\Delta=0.010 \mu\text{m}$, the new total film thickness, d_{Total} , would be

$$\begin{aligned}
d_{total} &= N_s \Delta \\
&= (16,384)(0.010) \\
&= 163.84 \text{ nm}
\end{aligned} \tag{A.3}$$

Using this new value for d_{Total} , the number of non-zero samples of the Q function for this parameter choice can be determined by

$$\begin{aligned}
N_0 &= d_{total} \left(\frac{1}{\lambda_i} - \frac{1}{\lambda_f} \right) \\
&= (163.84) \left(\frac{1}{0.58} - \frac{1}{0.62} \right) \\
&\Rightarrow 18 \text{ non - zero samples of } Q(k)
\end{aligned} \tag{A.4}$$

At this point the designer can decide to accept this set of parameters, or decide to try a different combination of values. For example, one might decide that 18 samples of the Q function is not enough, and decide to adjust the total thickness again to increase the number of samples. This would also affect the sample spacing of the index profile. To illustrate this, choose to keep the total number of samples $N_s=2^{14}=16,384$, but now choose to increase the total film thickness to be $d_{Total}=200 \text{ }\mu\text{m}$. Using this new value for d_{Total} , the number of non-zero samples of the Q function is

$$\begin{aligned}
N_0 &= d_{total} \left(\frac{1}{\lambda_i} - \frac{1}{\lambda_f} \right) \\
&= (200) \left(\frac{1}{0.58} - \frac{1}{0.62} \right) \\
&\Rightarrow 23 \text{ non - zero samples of } Q(k),
\end{aligned} \tag{A.5}$$

and the sample spacing in index, Δ , would be

$$\begin{aligned}
\Delta &= \frac{d_{total}}{N_s} \\
&= \frac{200}{16,384} \\
&= 0.0122 \text{ } \mu\text{m}
\end{aligned}
\tag{A.6}$$

This corresponds to an optical thickness sample spacing of 0.0061 μm , which is sufficient.

This collection of design parameters is closer to the original objectives, so they are selected to use in the example. The final parameters required as input to the programs in Appendix D are expressed in optical path length (not double optical path length). The conversion from optical path length to double optical path length is done in the programs as needed. The reason for this is to keep the input consistent with that required by the reflectance calculation. Therefore the final parameter values for total film thickness, d_{Total} , and sample spacing in index, Δ , are the values found above divided by 2. For the example of Section 3.3.1 the parameters are:

$$\begin{aligned}
N_s &= 2^{14} = 16,384 \\
d_{Total} &= 100 \text{ } \mu\text{m} \\
\Delta &= 0.0061 \text{ } \mu\text{m} \\
N_0 &\Rightarrow 23 \text{ non - zero samples of } Q
\end{aligned}
\tag{A.7}$$

This choice for the total optical thickness of the film should also minimize any aliasing effects, since it is over three times the desired film optical thickness. The same process is used to determine the parameters used in all of the examples in Chapter 3.

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Appendix C Vita

Captain Jeffrey J. Druessel was born on 15 October, 1963 in Decatur, Illinois. He graduated from Stephen Decatur High School in Decatur, Illinois in 1981, and continued his education at the University of Illinois at Urbana, Illinois, graduating in 1985 with a Bachelor of Science degree in Engineering Physics. He was commissioned in the United States Air Force in 1986 and was stationed at Vandenberg AFB, CA. During this tour he served as a weapons systems analyst for development testing of the Air Launched Anti-Satellite Missile, the Strategic Defense Initiative Space Based Interceptor Program, and the Peacekeeper and Small Intercontinental Ballistic missiles. In addition, he attended the University of Southern California extension at Vandenberg AFB, and graduated with a Master of Science in Systems Management in 1988. He married the former Joan M. Cairns of Lompoc, CA in April 1988. He entered the Air Force Institute of Technology School of Engineering in May 1990, and graduated with a Master of Science degree in Engineering Physics in 1991.

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APPENDIX A : SWIFT NUMERICAL DESIGN CONSIDERATIONS.....107

Figure A.1: Illustration of numerical parameters for discrete Fourier transform. 109

Appendix B : Optimization Theory

Introduction

The process of design requires a statement of the problem to be solved, identification of alternative solutions, and some measure of what constitutes a “best” solution to the problem. For simple problems, it may be possible to exhaustively list all possible solutions and “obviously” determine which one is best. For more complex problems, however, a more structured approach is needed to ensure the “best” solution is found. This structured approach consists of building a mathematical model for the system in question, identifying a set of variables to adjust in the design, and defining a “merit function” to numerically identify the best, or “optimal” solution. This section will summarize the theory of optimal design, which will be applied to the problem of gradient index thin film design in Chapter 4.

Statement of Optimal Design Problem

To express a design problem in mathematical form, one first must define the physical system to be modeled and identify the inputs to and outputs from this system. The next step is to construct a mathematical model of the system which approximates its performance by correctly mapping inputs to outputs. The model consists of a set of design variables and a collection of functions of these variables that define the objective and the constraints on the problem. The objective function (sometimes referred to as the merit function) is usually constructed such that its minimum value represents the optimal

design. The formal definition of the constrained optimization problem with n real-valued variables is therefore

$$\begin{array}{ll}
 \text{minimize} & f(\mathbf{x}) \\
 & \mathbf{x} \in \mathcal{R}^n \\
 \text{Subject to:} & \\
 & g_i(\mathbf{x}) = 0 \quad i = 1, 2, \dots, m_e \\
 & g_j(\mathbf{x}) \leq 0 \quad j = m_e + 1, \dots, m \\
 & \mathbf{x}_{\min} \leq \mathbf{x} \leq \mathbf{x}_{\max}
 \end{array} \tag{B.1}$$

where \mathbf{x} is a vector of the design variables, $f(\mathbf{x})$ is the objective function, the $g_i(\mathbf{x})$'s are the constraint functions, and the \mathbf{x}_{\min} and \mathbf{x}_{\max} are vector bounds on the design variables. It should be noted here that there are two general classes of constrained optimization problems. The first class is characterized by the fact that all the functions in Equation B.1 are linear functions of the design variables. This class of problems can be readily solved by the techniques of linear programming. The second class of problems, and the one with which the rest of this paper is concerned, have non-linear functions of the design variables as objective functions or constraints. This format of the optimal design problem with the constraints all expressed as less than or equal to zero is called the Null Negative Form [28:17]. The solution of the problem expressed by Equation B.1 is denoted by \mathbf{x}^* .

A few additional definitions/concepts are needed before describing the methods used to solve the optimal design problem. First, a point \mathbf{x}_o in the vector space \mathcal{R}^n is a "feasible" point if all constraints $g_i(\mathbf{x}_o)$ are satisfied by equality or inequality, as required by the constraint. Conversely, a point in \mathcal{R}^n where this is not true is called an "infeasible" point. The second concept is that of "active" constraints. A constraint is said to be active if it is equal to zero when evaluated at the solution point ($g_i(\mathbf{x}^*)=0$). Clearly, all equality constraints are active by definition.

Now that the mathematical problem has been defined, how is a solution determined? Conceptually, the most straightforward method would be to select a feasible point x_k in the vector space \mathcal{R}^n as a start, then explore the neighborhood by adjusting each element of the vector by a fixed amount. Then evaluate the objective function and constraints at each test point, and identify the feasible point for which the objective function is smallest. This test point would become the new starting point, x_{k+1} , and the procedure would be repeated until a minimum value for the objective function is found. While this method is easily visualized, it is not practical. There are much more efficient techniques for determining the solution to the constrained optimal design problem. The current state of the art in non-linear optimization is a method known as Sequential Quadratic Programming (SQP) [28:365-372]. The basic theory for this method is outlined below.

Kuhn-Tucker Conditions and SQP

The general approach to solving non-linear constrained optimization problems is to transform the problem into an easier sub-problem, which can be iterated to find the true solution. The foundation of this approach is a set of necessary conditions on the solution of a general constrained optimization problem known as the Kuhn-Tucker (KT) equations: [26:2-22]

$$\begin{aligned} \nabla f(x^*) + \sum_{i=1}^m \lambda_i^* \nabla g_i(x^*) &= 0 \\ \lambda_i^* g_i(x^*) &= 0 \quad i = 1, \dots, m \\ \lambda_i^* &\geq 0 \quad i = m_e + 1, \dots, m \end{aligned} \tag{B.2}$$

The first equation is the gradient of the Lagrangian, and describes a canceling of the gradients between the objective function, f , and the constraints, g_i , weighted by Lagrange multipliers, λ_i . Only active constraints are included in this expression, so the Lagrange multiplier for any inactive constraint is set to zero. The solution point \mathbf{x}^* is assumed to be a "regular" point, which means that gradients of the constraints are linearly independent at that point. Note that the KT equations are not sufficient conditions for a solution, so each point which satisfies Equation B.2 must be checked individually to determine if it is the optimal solution. An additional sufficiency condition can be formed using information on the second derivative of the Lagrangian. For any regular solution point of the KT equations, \mathbf{x}^* , if the Hessian of the Lagrangian at \mathbf{x}^* is positive-definite, then the solution point is a local constrained minimum [28:184]. A positive-definite matrix is symmetric and has only positive, real elements. The mathematical expressions for the Lagrangian (denoted by L) and the Hessian of the Lagrangian (denoted by H), are given below:

$$L(\mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{x}) + \sum_{i=1}^m \lambda_i g_i(\mathbf{x}), \quad \mathbf{x} = (x_1, x_2, \dots, x_n)$$

$$H(\mathbf{x}, \boldsymbol{\lambda}) = \begin{bmatrix} \frac{\partial^2 L}{\partial x_1 \partial x_1} & \frac{\partial^2 L}{\partial x_1 \partial x_2} & \dots & \frac{\partial^2 L}{\partial x_1 \partial x_n} \\ \frac{\partial^2 L}{\partial x_2 \partial x_1} & \frac{\partial^2 L}{\partial x_2 \partial x_2} & & \\ \vdots & & \ddots & \vdots \\ \frac{\partial^2 L}{\partial x_n \partial x_1} & \dots & \dots & \frac{\partial^2 L}{\partial x_n \partial x_n} \end{bmatrix} \quad (\text{B.3})$$

These necessary and sufficient conditions for the solution of the original constrained optimization problem can be used in building a sequence of easier sub-problems to solve.

The easier sub-problem to be solved is to determine the best “direction” in the vector space of variables to move in for the next iteration, as well as the length of step to take along this direction. Again using the null negative form of the problem in Equation B.1, form the Lagrangian as

$$L(\mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{x}) + \sum_{i=1}^m \lambda_i g_i(\mathbf{x}) \quad (\text{B.4})$$

The simplified problem, called the Quadratic Programming (QP) sub-problem, is to solve the quadratic approximation to the Lagrangian above subject to linearized constraints [28:367]. The quadratic approximation to the Lagrangian is found by expanding in a Taylor’s series and keeping terms up to second order in \mathbf{x} . For any fixed point in the vector space of variables, \mathbf{x}_k , the QP sub-problem can be written as

$$\begin{array}{ll} \text{minimize} & \frac{1}{2} \mathbf{d}^T \mathbf{H} \mathbf{d} + \nabla f(\mathbf{x}_k)^T \mathbf{d} \\ \text{subject to:} & \\ & \nabla g_i(\mathbf{x}_k)^T \mathbf{d} + g_i(\mathbf{x}_k) = 0, \quad i = 1, 2, \dots, m_e \\ & \nabla g_i(\mathbf{x}_k)^T \mathbf{d} + g_i(\mathbf{x}_k) \leq 0, \quad i = m_e + 1, \dots, m \end{array} \quad (\text{B.5})$$

Here the functions f and g_i are the original objective function and constraints, \mathbf{H} is a positive-definite approximation to the Hessian of the Lagrangian, and \mathbf{d} is the new step direction for the next iteration. Bold typeface indicates a vector or matrix. The superscript T indicates matrix transpose. The solution to this QP sub-problem is used to determine the next iteration point $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha \mathbf{d}$, where the step length α is to be determined. The step length α is needed to stabilize the algorithm, because it is possible

that the solution to the QP sub-problem is infeasible. It is found by performing a line search along the direction d and minimizing a merit function, which includes penalties for infeasible solutions.

In summary, the SQP algorithm is:

1. Select a starting point, x_0 , and an initial estimate for λ_0 . ($k=0$)
2. Solve the QP sub-problem above to determine the step direction d and the new estimate of λ_{k+1} . ($k=k+1$)
3. Set $x_{k+1} = x_k + \alpha d$.
4. Test for termination. If criteria not satisfied, goto step 2.

The SQP algorithm for solution of non-linear optimization problems is available in the MATLAB™ Optimization Toolbox [26, 27]. MATLAB™ is an interactive software package for scientific and engineering numeric computation [27:4]. The next section outlines the numerical methods used by MATLAB™ to implement this algorithm.

MATLAB™ Implementation of SQP

The numerical optimizations performed in this research were done using the MATLAB™ software package and in particular the MATLAB™ optimization toolbox [26,27]. The MATLAB™ software uses the SQP algorithm described above in its constrained optimization routines. To implement the theory above, the program must estimate the gradients and the Hessian at each point. The implementation of the SQP is done in three main stages [26:2-26]:

1. Update the estimate for the Hessian matrix of the Lagrangian.
2. Solve the QP sub-problem.
3. Perform line search and merit function minimization.

Equality vs. Inequality Constraints

The MATLAB™ algorithm differentiates between equality and inequality constraints. Equality constraints are active by definition, and have non-zero Lagrange multipliers. Inequality constraints are included in null negative form, and may or may not be active. The program uses an active set strategy approach to handle the inequality constraints. This means that an estimate of which constraints are active is calculated at each iteration. This estimate of activity figures in the merit function used in the determination of step size. Also, the zero tolerances for the equality and inequality constraints are controlled separately. This can impact the results, depending on how the problem is originally stated.

Gradient Estimation

If the objective functions and constraints are not known analytically, the partial derivatives needed to estimate the gradients must be calculated numerically. MATLAB™ uses an adaptive finite difference technique to find the values of the gradients as needed. The maximum and minimum perturbations for this calculation can be controlled by the user.

BFGS Method for Hessian Estimation

The key to the SQP algorithm is knowledge of the Hessian of the Lagrangian for the problem. Since this matrix is computationally expensive to calculate directly, it is estimated and refined through iteration using the formula devised by Broyden, Fletcher, Goldfarb, and Shanno (BFGS) [26:2-26]. In addition, the estimate for the Hessian is forced to remain positive-definite, so the solution to the original problem is a minimum.

Termination Criteria

The optimization goal is achieved when three termination criteria have been satisfied. There are three numerical tolerances to be met, one on the objective function, one on the variables, and one on the constraints. The objective function tolerance specifies the precision required on the objective function at the solution. The termination criteria for variables specify the minimum acceptable precision on the values of the variables. The constraint termination criterion is the maximum allowable violation of the constraints at the solution point. All three termination criteria must be satisfied simultaneously to achieve an optimal solution. The default termination tolerances are: objective -- 10^{-4} , variables -- 10^{-4} , and constraints -- 10^{-7} . All three can be adjusted if necessary.

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Appendix C Vita

Captain Jeffrey J. Druessel was born on 15 October, 1963 in Decatur, Illinois. He graduated from Stephen Decatur High School in Decatur, Illinois in 1981, and continued his education at the University of Illinois at Urbana, Illinois, graduating in 1985 with a Bachelor of Science degree in Engineering Physics. He was commissioned in the United States Air Force in 1986 and was stationed at Vandenberg AFB, CA. During this tour he served as a weapons systems analyst for development testing of the Air Launched Anti-Satellite Missile, the Strategic Defense Initiative Space Based Interceptor Program, and the Peacekeeper and Small Intercontinental Ballistic missiles. In addition, he attended the University of Southern California extension at Vandenberg AFB, and graduated with a Master of Science in Systems Management in 1988. He married the former Joan M. Cairns of Lompoc, CA in April 1988. He entered the Air Force Institute of Technology School of Engineering in May 1990, and graduated with a Master of Science degree in Engineering Physics in 1991.

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Appendix C : Wavelet Theory

Wavelets are a relatively new mathematical technique. They are a form of generalized Fourier series, using wavelets as basis elements instead of sines and cosines. These new basis elements will be used to solve Maxwell's equations for the fields inside the film, and establish a new form for the mapping between index of refraction and reflectivity. The sections below will first introduce some of the basic concepts of wavelets, and then describe the technique of multi-resolution analysis.

Basic Wavelet Concepts

The term wavelets was first coined in 1982 by Morlet, who used a mathematical technique similar to Fourier series but using "little waves" as the basis elements, instead of sines and cosines [8:2]. The wavelets must be oscillatory (the wave part) and must also decay rapidly (the little part). An example of such a wavelet, called the Morlet wavelet, is shown in Figure C.1.

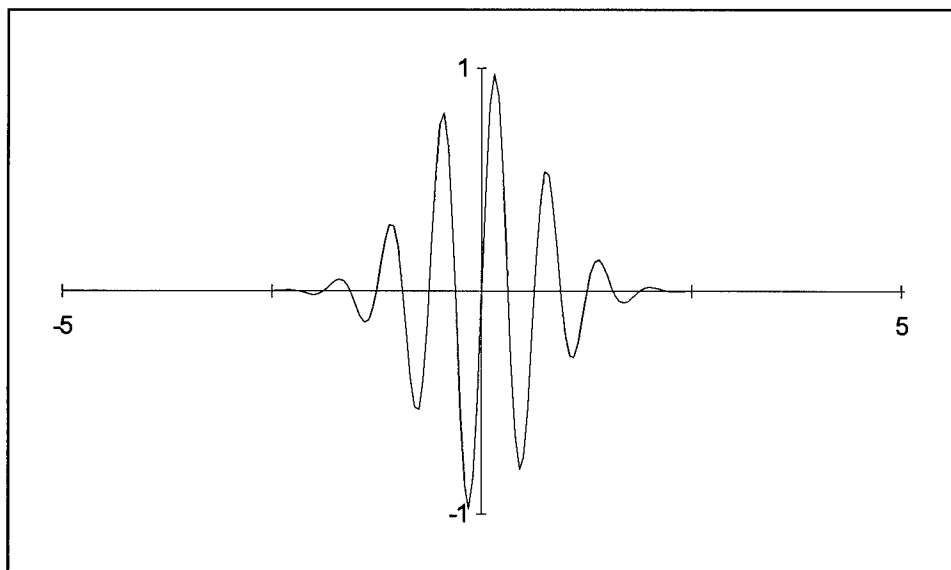


Figure C.1: Morlet Wavelet

In Fourier analysis the pieces used to decompose and reconstruct a signal are sines and cosines of different frequencies. In wavelet analysis the building blocks are translated and dilated (shifted and scaled) versions of a single wavelet, called the “mother wavelet” [46:2]. Denoting the mother wavelet by $h(t)$, the rest of the building blocks are given by

$$h_{a,b}(t) = \frac{1}{\sqrt{|a|}} h\left(\frac{t-b}{a}\right) \quad (\text{C.1})$$

where a is the scale and b is the shift [7:909]. The mother wavelet h must satisfy the condition

$$\int_{-\infty}^{\infty} h(x) dx = 0 \quad (\text{C.2})$$

which implies that $\hat{h}(0) = 0$, where the $\hat{}$ denotes Fourier transform. If the shift b and scale a vary continuously, the continuous wavelet transform based on this mother wavelet, h , maps a one dimensional function $f(x)$ to a two dimensional surface $W_h f(a,b)$. The mathematical form of this transform is

$$W_h f(a,b) = \int_{-\infty}^{\infty} f(x) h_{a,b}(x) dx \quad (\text{C.3})$$

If the shift and scale are restricted to a discrete sublattice, the continuous wavelet transform above becomes a discrete wavelet transform. The wavelets become [7:910]

$$h_{m,n}(t) = a_0^{-m/2} h(a_0^{-m} t - n b_0) \quad m, n \in \mathbb{Z} \quad (\text{C.4})$$

where

$$\begin{aligned} a &= a_0^m \\ b &= n b_0 a_0^m \end{aligned} \quad (\text{C.5})$$

\mathbb{Z} is the set of integers

For this work it is convenient to choose $a_0=2$, and $b_0=1$, although other choices are possible. With this choice of a_0 and b_0 it is possible to construct an $h(t)$ such that $h_{m,n}$ form an orthonormal basis for $L^2(\mathfrak{R})$ [7:911], where $L^2(\mathfrak{R})$ is the set of all measurable functions of finite energy, defined by

$$L^2(\mathfrak{R}) = \left\{ f : f \text{ is measurable and } \int_{-\infty}^{\infty} |f(x)|^2 dx < \infty \right\} \quad (\text{C.6})$$

Multiresolution Analysis

A multiresolution analysis is a technique of representing a function $f \in L^2(\mathfrak{R})$ as a limit of successive approximations, each of which is a smoothed version of f [7:913, 25]. A multiresolution analysis consists of: [7:915, 45:152-158]

(i.) A group of embedded subspaces $V_m \subset L^2(\mathfrak{R})$, such as

$$\dots \subset V_2 \subset V_1 \subset V_0 \subset V_{-1} \subset V_{-2} \dots \quad (\text{C.7})$$

(ii.) These subspaces have only the zero element in common, and the sum of the spaces span all of $L^2(\mathfrak{R})$:

$$\bigcap_{m \in \mathbb{Z}} V_m = \{0\} \quad \overline{\bigcup_{m \in \mathbb{Z}} V_m} = L^2(\mathfrak{R}) \quad (\text{C.8})$$

(iii.) If a function is an element of one space, then the same function scaled by a factor of 2 is an element of the next higher space:

$$f(x) \in V_m \quad f(2x) \in V_{m-1} \quad (\text{C.9})$$

(iv.) There exists a function $\phi \in V_0$ such that shifted versions of this function form a basis for the space V_0 :

$$\begin{aligned} V_0 &= \overline{\text{span}\{\phi_{0,n}, n \in \mathbb{Z}\}} \\ \phi_{m,n}(t) &= 2^{-m/2} \phi(2^{-m}t - n) \end{aligned} \quad (\text{C.10})$$

The first property above means that any feature that can be seen at coarse resolution (like V_1) can also be seen at finer resolutions (like V_0). Naturally, the finer resolutions also contain more detailed features as well. The second property describes the limits of this ladder of subspaces. At the coarsest resolution there is nothing left but the zero element of the space, while in the limit of the finest resolution the V_m converge to $L^2(\mathbb{R})$. The third property is the same scaling feature already identified as a property of wavelets. The last property is the building block for the analysis. For a fixed dilation (scale), translations (shifts) of the function ϕ are basis elements for that subspace. These functions ϕ are called scaling functions, or father wavelets. Only real scaling functions will be considered here, although complex ϕ are possible.

Since a space V_m has a basis given by $\phi_{m,n}$, then any element of the space can be written as a linear combination of these basis elements. That is if $x(t) \in V_m$, then there exist coefficients $c_{m,n}$ such that

$$\begin{aligned} x(t) &= \sum_{n \in \mathbb{Z}} c_{m,n} 2^{-m/2} \phi(2^{-m}t - n) \\ &= \sum_{n \in \mathbb{Z}} c_{m,n} \phi_{m,n}(t) \end{aligned} \quad (\text{C.11})$$

The $c_{m,n}$ are called approximation coefficients. They are found by taking the inner product of the function $x(t)$ with the scaling function $\phi_{m,n}$

$$\begin{aligned} c_{m,n} &= \int_{-\infty}^{\infty} x(t) \phi_{m,n}(t) dt \\ &= \langle x, \phi_{m,n} \rangle. \end{aligned} \quad (\text{C.12})$$

The Dirac bracket notation is used to denote the inner product of two functions. For $f \in L^2(\mathbb{R})$, a projection operator P_m can be defined by

$$P_m f = \sum_{n \in \mathbb{Z}} \langle f, \phi_{m,n} \rangle \phi_{m,n} \quad (\text{C.13})$$

which gives the expression for that part of $f(t)$ that is an element of V_m . Since all the elements in V_m are in V_{m-1} (by the construction of the ladder of subspaces), what elements are in V_{m-1} that are not in V_m ? Construct a projection operator Q_m that identifies such elements by

$$Q_m f = P_{m-1} f - P_m f \quad (\text{C.14})$$

By the Classical Projection Theorem, the $Q_m f$ is orthogonal to V_m , and so defines a space of all such elements, called W_m , whose inner product with elements of V_m is zero. In set notation, that is [45:162]

$$W_m = \{ f \in V_{m-1} : \langle f, v \rangle = 0 \ \forall \ v \in V_m \} \quad (\text{C.15})$$

So by definition of W_m and Q_m

$$\begin{aligned}
 P_{m-1}f &= P_m f + Q_m f \\
 \text{c} \\
 V_{m-1} &= V_m \oplus W_m
 \end{aligned}
 \tag{C.16}$$

where the symbol “ \oplus ” is the orthogonal direct sum of the two spaces. The direct sum is the set of vectors formed by adding one element from each of the orthogonal subspaces. Equation C.16 is a key point in the multiresolution analysis theory. Each subspace V_{m-1} consists of the direct sum of two other subspace, V_m and W_m . This idea is illustrated graphically in Figure C.2.

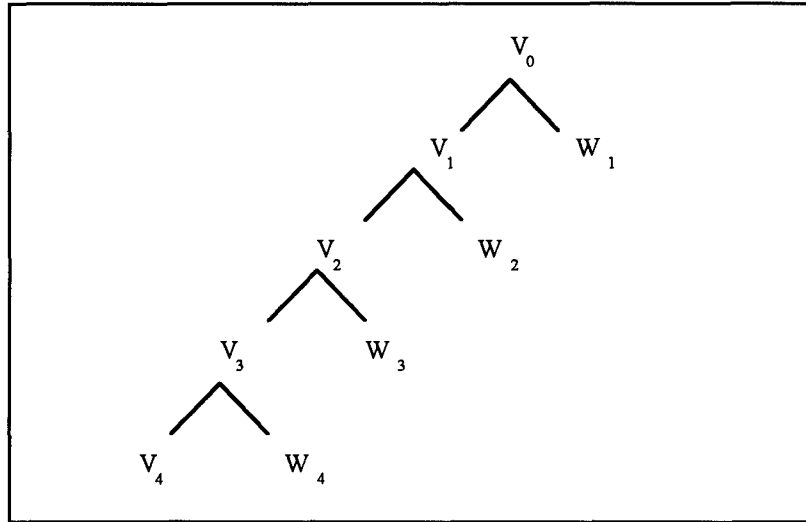


Figure C.2: Structure of Nested Subspaces

By the nature of the ladder of subspaces and the fact that W_m is orthogonal to V_m , the W_m 's are all mutually orthogonal. Furthermore, the combination of all the W_m 's spans the entire space of $L^2(\mathfrak{R})$ functions:

$$\bigoplus_{m \in \mathbb{Z}} W_m = L^2(\mathfrak{R})
 \tag{C.17}$$

Now identify the basis for each W_m as $\{ \Psi_{m,n} : n \in \mathbb{Z} \}$. This set of functions forms a basis for the entire space $L^2(\mathcal{R})$, and they are the wavelets we seek. The details of the techniques used to construct the scaling function $\phi_{m,n}$ and the wavelets $\Psi_{m,n}$ are not necessary to understand the use of this theory. Several different types of scaling functions and wavelets have been developed in the literature. These include the Haar basis above, which is the simplest, as well as Daubechies' compactly supported wavelets [7:980]. Illustrations of some of Daubechies' wavelets and their associated scaling functions are shown in Figure C.3. The different wavelet-scaling function pairs shown are labeled by the number of filter coefficients, or "taps", needed to completely specify each wavelet. The functional form of the scaling functions and wavelets are not required to implement the method of multiresolution analysis, as will be seen in the next section.

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Figure C.3: Illustration of Daubechies' compactly supported wavelets and scaling functions: (a) 2 tap (Haar), (b) 4 tap, (c) 8 tap, (d) 16 tap.

Function Decomposition and Reconstruction

To make use of the multiresolution analysis theory, a method is needed to represent the function to be analyzed in each of the subspaces, preferably without performing numerous integrations. To develop such a method, define the coefficients of expansion for each level “ m ” by

$$P_m f(t) = \sum_{n \in \mathbb{Z}} c_{m,n} \phi_{m,n}(t) \quad (\text{C.18})$$

$$Q_m f(t) = \sum_{n \in \mathbb{Z}} d_{m,n} \psi_{m,n}(t)$$

The coefficients $c_{m,n}$ are found by taking the inner product of the projection of $f(t)$ onto V_m with the scaling function $\phi_{m,n}$. Applying the relationship between the projection operators in Equation C.17 to this expression for $c_{m,n}$ yields

$$\begin{aligned} c_{m,n} &= \langle P_m f, \phi_{m,n} \rangle \\ &= \langle P_{m-1} f, \phi_{m,n} \rangle - \langle Q_m f, \phi_{m,n} \rangle \end{aligned} \quad (\text{C.19})$$

However, the second inner product is zero because $Q_m f(t) \perp \phi_{m,n}$ by construction. This leaves a recursive relationship between the coefficients:

$$c_{m,n} = \sum_{\ell \in \mathbb{Z}} c_{m-1,\ell} \langle \phi_{m-1,\ell}, \phi_{m,n} \rangle \quad (\text{C.20})$$

Similarly for $d_{m,n}$

$$\begin{aligned}
d_{m,n} &= \langle Q_m f, \psi_{m,n} \rangle \\
&= \langle P_{m-1} f, \psi_{m,n} \rangle - \langle P_m f, \psi_{m,n} \rangle \\
&= \sum_{\lambda \in \mathbb{Z}} c_{m-1,\lambda} \langle \phi_{m-1,\lambda}, \psi_{m,n} \rangle.
\end{aligned} \tag{C.21}$$

The recursive relations above show all that is needed to decompose a function is to find the inner products between a scaling function and the scaling function or wavelet of the next level down. Consider the explicit form of one of these inner products

$$\langle \phi_{m-1,\ell}, \phi_{m,n} \rangle = 2^{-(m-1)/2} 2^{-m/2} \int_{-\infty}^{\infty} \phi(2^{-(m-1)}t - \ell) \phi(2^{-m}t - n) dt \tag{C.22}$$

Let $\frac{u}{2} = 2^{-m}t - n$. Then

$$\langle \phi_{m-1,\ell}, \phi_{m,n} \rangle = 2^{-1/2} \int_{-\infty}^{\infty} \phi\left(\frac{u}{2}\right) \phi(u - [\ell - 2n]) du \tag{C.23}$$

Define a sequence $h(n)$ by

$$h(n) \doteq 2^{-1/2} \int_{-\infty}^{\infty} \phi\left(\frac{t}{2}\right) \phi(t - n) dt \tag{C.24}$$

then

$$\langle \phi_{m-1,\lambda}, \phi_{m,n} \rangle = h(\lambda - 2n) \tag{C.25}$$

Notice this relation is **independent of the level m !** This means that the coefficients for any level can be found from the coefficients for the level above. (Also note the sequence $h(n)$ defined in Equation C.25 above is not related to the wavelet $h(t)$ defined in the previous section. This conflicting notation is standard within the wavelet

literature.) The coefficients required to specify the Daubechies' wavelets shown in Figure C.3 are listed in Table C-1.

Table C-1: Daubechies' wavelet coefficients [7:980]

h=2: 0.7071067811865	h=16: 0.054415842243
0.7071067811865	0.312871590914
	0.675630736297
h=4: 0.482962913145	0.585354683654
0.836516303738	-0.015829105256
0.224143868042	-0.284015542962
-0.129409522551	0.000472484574
	0.128747426620
h=8: 0.230377813309	-0.017369301002
0.714846570553	-0.044088253931
0.630880767930	0.013981027917
-0.027983769417	0.008746094047
-0.187034811719	-0.004870352993
0.030841381836	-0.000391740373
0.032883011667	0.000675449406
-0.010597401785	-0.000117476784

Thus, there is a recursion relation between levels that can be exploited to calculate the coefficients:

$$c_{m,n} = \sum_{\ell \in \mathbb{Z}} c_{m-1,\ell} h(\ell - 2n) \quad (\text{C.26})$$

A similar relation exists for the detail coefficients, $d_{m,n}$:

$$\begin{aligned} \langle \phi_{m-1,\ell}, \psi_{m,n} \rangle &= g(\ell - 2n) \\ g(n) &= 2^{-1/2} \int_{-\infty}^{\infty} \psi\left(\frac{t}{2}\right) \phi(t - n) dt \end{aligned} \quad (\text{C.27})$$

$$d_{m,n} = \sum_{\ell \in \mathbb{Z}} c_{m-1,\ell} g(\ell - 2n)$$

The decomposition algorithm in this multiresolution analysis requires only the filters h and g to define the wavelets to be used. In fact, the g filter can be derived from the h filter, so only one sequence is needed to completely determine the wavelets. This relationship between h and g is

$$g(n) = (-1)^n h(n - 1) \quad (\text{C.28})$$

Using the two recursion relations for $c_{m,n}$ and $d_{m,n}$, any function can be decomposed into its approximation and detail coefficients from an initial sequence c_0 . Figure C.4 illustrates the relationship between these coefficients. Note the structure of the coefficients is the same as the structure of the underlying spaces, V_m and W_m .

Now that the technique used to decompose a function has been identified, how is the original function reconstructed from these coefficients? As can be seen from Figure C.4, only the coarsest (lowest) approximation coefficient and the detail coefficients are needed to reconstruct the original c_0 .

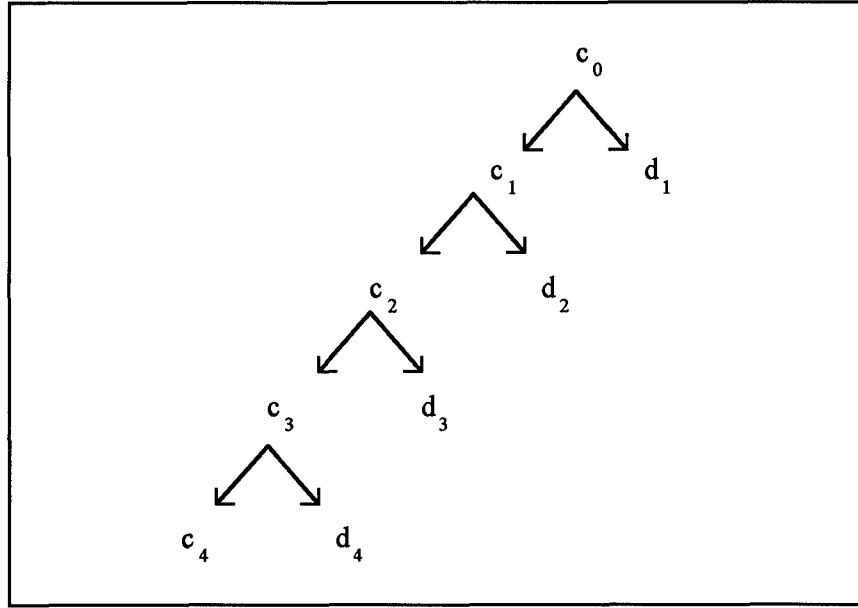


Figure C.4: Wavelet decomposition tree.

The recursive relation for reconstruction is

$$c_{m-1,k} = \sum_{n \in \mathbb{Z}} c_{m,n} h(k-2n) + \sum_{n \in \mathbb{Z}} d_{m,n} g(k-2n) \quad (\text{C.29})$$

A further simplification to the decomposition-reconstruction algorithm can be made by treating the initial sequence of coefficients as part of a periodic sequence. Wavelet transforms have the property that the transform of a periodic function is also periodic. In the case of the multiresolution decomposition, if the top sequence c_0 has N values, and N is a power of 2 (i.e., $N=2^M$ for some integer M), then the next level coarse coefficients c_1 will be 2^{M-1} periodic, as will the details for that level, d_1 . So the lowest level of decomposition consists of a 1-periodic coarse coefficient sequence (a constant), and a 1-periodic detail coefficient sequence.

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Appendix D Vita

Captain Jeffrey J. Druessel was born on 15 October, 1963 in Decatur, Illinois. He graduated from Stephen Decatur High School in Decatur, Illinois in 1981, and continued his education at the University of Illinois at Urbana, Illinois, graduating in 1985 with a Bachelor of Science degree in Engineering Physics. He was commissioned in the United States Air Force in 1986 and was stationed at Vandenberg AFB, CA. During this tour he served as a weapons systems analyst for development testing of the Air Launched Anti-Satellite Missile, the Strategic Defense Initiative Space Based Interceptor Program, and the Peacekeeper and Small Intercontinental Ballistic missiles. In addition, he attended the University of Southern California extension at Vandenberg AFB, and graduated with a Master of Science in Systems Management in 1988. He married the former Joan M. Cairns of Lompoc, CA in April 1988. He entered the Air Force Institute of Technology School of Engineering in May 1990, and graduated with a Master of Science degree in Engineering Physics in 1991.

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